

Quantum Monte Carlo simulations of bosonic and fermionic impurities in a two-dimensional hard-core boson system

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(Dated: February 1, 2008)

A two-dimensional lattice hard-core boson system with a small fraction of bosonic or fermionic impurity particles is studied. The impurities have the same hopping and interactions as the dominant bosons and their effects are solely due to quantum statistics. Quantum Monte Carlo simulations are carried out in which paths of the dominant boson species are sampled and a summation is performed over all second-species paths compatible with the permutation cycles. Both kinds of impurities reduce modestly and equally the Kosterlitz-Thouless superfluid transition temperature. However, the effective impurity interactions are found to be qualitatively different at lower temperatures; fermions are repulsive and further suppress superfluidity as $T \rightarrow 0$.

PACS numbers: 03.75.Mn, 03.75.Hh, 05.30.Fk, 05.10.Ln

Ultracold atoms in optical lattices offer unprecedented opportunities to realize novel quantum states of matter [1]. One prospect is to tailor systems to mimic hamiltonians of fundamental interest in condensed matter physics, e.g., the Hubbard model [2]. Another interesting route is to explore states that do not have any realizations in naturally occurring systems. The use of mixtures of different atomic species open up almost endless possibilities. In the case of two species, there are three mixture classes; bose-bose, fermi-fermi, and bose-fermi, with the latter perhaps offering the most interesting prospects. Several exotic phases have been predicted theoretically, e.g., supersolids [3], several different Mott states [4], multiply degenerate quantum-disordered states with glass-like properties [5], paired states with various orbital symmetry [6], and a host of states of effective fermion-boson composite particles [7]. Experimentally, there are intriguing results indicating a strong influence of a small admixture of fermions in boson gases in optical lattices [8].

In this Letter a simple two-species model will be considered in which all particles have identical hoppings and interactions, posing a clean way to elucidate the fundamental role of quantum statistics. The situation can be realized experimentally in systems with two isotopes of the same atom, e.g., ^6Li - ^7Li mixtures [9]. A 1D model of this kind has been studied using various analytical approaches [10]. Here a quantum Monte Carlo (QMC) method is developed for a low concentration of fermionic or bosonic impurities in a bath of bosons. The scheme is applied to a 2D model. Defining creation operators a_i^\dagger and b_i^\dagger for the two species the hamiltonian is

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i + b_i^\dagger b_j + b_j^\dagger b_i), \quad (1)$$

where $\langle ij \rangle$ denotes nearest neighbors on a square lattice of $N = L \times L$ sites with periodic boundaries. Species A is bosonic, whereas the B particles can be either bosons or fermions. Both are subject to a hard-core constraint, i.e., the sites are either empty or singly-occupied. Half-filling

in the canonical ensemble will be considered here; $n = n_A + n_B = N/2$, where $n_A = \sum a_i^\dagger a_i$ and $n_B = \sum b_i^\dagger b_i$. The trapping potential necessary to model experiments is left out, but can easily be incorporated in future work using the QMC scheme introduced below.

With a fermionic B species, the hamiltonian as a function of n_B/n interpolates between spinless fermions and the standard hard-core boson model, which is equivalent to the $S = 1/2$ XY model and undergoes a Kosterlitz-Thouless (KT) transition to a superfluid with power-law off-diagonal correlations at temperature $T_{\text{KT}}/t \approx 0.69$ [11]; at $T = 0$ it is long-range ordered. The spinless fermion model, on the other hand, has a metallic ground state and does not undergo any finite- T transition. It is then interesting to consider the evolution of the ground state and finite- T properties as a function of the fermion fraction. Here the A species will be considered dominant, the B particles acting as impurities; $n_B \ll n_A$.

The purely bosonic ground state does not change when some A particles are replaced by another boson species. The excitations are affected, however, and one can expect a reduction in T_{KT} relative to the single-species system. It will be shown here that the effective interaction between the impurities is attractive at high temperatures but changes, in a singular way, to repulsive at T_{KT} . Bosonic impurities become attractive at lower T , whereas fermions stay repulsive as $T \rightarrow 0$. The effects of the impurities on the KT transition are independent of their statistics, but there are indications of a more dramatic suppression of superfluidity by fermions as $T \rightarrow 0$.

QMC Algorithm.—Consider finite- T QMC methods in which the density matrix $e^{-H/T}$ ($k_B = 1$) is written as a sum of operators P_i which propagate real-space states $|\alpha\rangle$ such that $P_i|\alpha\rangle = W_i(\alpha)|\alpha\rangle$. The paths (i, α) are importance-sampled according to their weights $W_i(\alpha)$ in the partition function $Z = \sum_{i, \alpha} W_i(\alpha)$. Such path-integral methods based on "time-slicing" can be formulated in the continuum [12] and on lattices [13]. In recent years very efficient algorithms for updating the paths

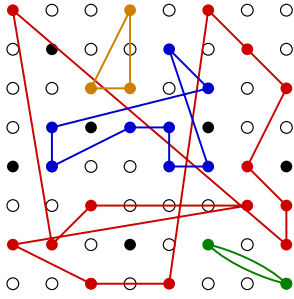


FIG. 1: (Color online) Permutation cycles for an 8×8 system at $T/t = 0.5$. Open and solid circles represent empty sites and particles, respectively. The net effect of the SSE propagation of the state is to cyclically permute the particles connected by the closed paths. The isolated solid (black) circles are particles not undergoing any net permutations; they are considered permutation cycles of length one.

have been devised [14, 15, 16] and systems with thousands of bosons can now be routinely simulated even at low temperatures. On the lattice, the alternative stochastic series expansion (SSE) approach [15, 17, 18], in which $e^{-H/T}$ is Taylor expanded to all contributing orders, is often more efficient and will be employed here. The details of the method are unimportant, however, and the scheme for treating impurity particles outlined below should be applicable with any standard boson QMC algorithm.

Identical particles in $P_i|\alpha\rangle$ are permutations of those in $|\alpha\rangle$. The permutations can be decomposed into cycles C_i in which m_i particles are permuted independently of the other particles. An example from an actual SSE simulation of an 8×8 lattice with 32 bosons is shown in Fig. 1. In the case of a multi-species system, a term (path) contributes to the partition function as long as all particles within each individual permutation cycle are identical; particles in different cycles do not have to be identical. Now, if all the interaction and hopping parameters are identical for all species, the weight $W_i(\alpha)$ is independent of the (allowed) distributions of the particles over the cycles. A simulation can then be carried out for all identical hard-core bosons (A particles) and, subsequently, when measuring observables, two (or more) species can be considered by substituting all the particles in some of the cycles with B particles. All ways of filling the cycles can be summed up exactly, including fermionic signs.

Denote by $N_c(m)$ the number of cycles of length m and by $n_c(m)$ the number of cycles filled with B particles. Then the total number of ways of distributing n_b bosons of type B in the system (substituting the same number of A particles) is given by

$$w_b = \sum_{\{n_c\}} \prod_{m=1}^{n_b} \binom{N_c(m)}{n_c(m)}, \quad (2)$$

where, for a fixed number n_b of B particles, the sum is over all cycle fillings satisfying the constraint $\sum_m m n_c(m) = n_b$. Thus, if the paths are importance-

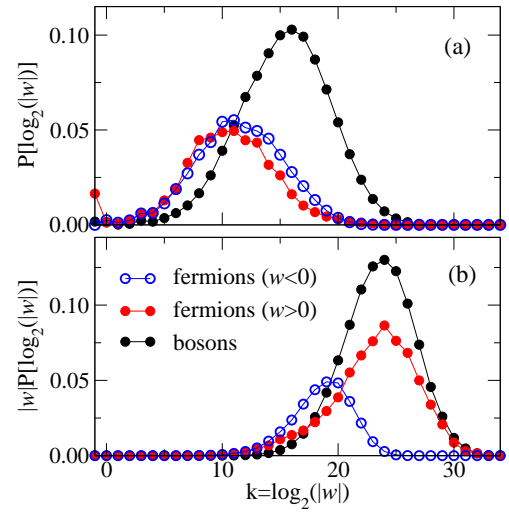


FIG. 2: (Color online) (a) Weight distribution for fermions ($w_f \geq 0$ and $w_f < 0$ separately) and bosons in simulations of an $L = 16$ lattice with $n_{b,f} = 12$ at $T/t = 0.25$. Bin k (integer) represents the probability of $k \leq \log_2(|w|) < k + 1$ (the special case $w = 0$ is in the $k = -1$ bin). (b) The probability times the weight, i.e., the actual contribution of terms in a given weight range (normalized to unity for both bosons and fermions). The scheme breaks down when a significant fraction of the weight in a histogram in (b) extends far into the rarely sampled right tail of the probability histogram in (a). Here the average fermionic sign, i.e., the ratio of fermionic and bosonic weights, $\langle S \rangle = \langle w_f \rangle / \langle w_b \rangle \approx 0.03$. The effective sign in the simulation is the difference between the $w_f \geq 0$ and $w_f < 0$ histograms in (b) and is larger; $\langle S \rangle_{\text{eff}} \approx 0.4$

sampled using the weight $W_i(\alpha)$, the measurements of some observable \hat{O} should be weighted by w_b ;

$$\langle \hat{O} \rangle = \frac{\sum_{i,\alpha} w_b(i, \alpha) \langle O_{i,\alpha} \rangle}{\sum_{i,\alpha} w_b(i, \alpha)}. \quad (3)$$

Here the sums are over the paths actually sampled in the simulation. The estimator $\langle O_{i,\alpha} \rangle$ is an average over the $w_b(i, \alpha)$ different cycle fillings.

In the case of fermions, each cyclic permutation of an even number of particles yields a minus sign. Thus, in the presence of n_f fermionic B particles the weight is

$$w_f = \sum_{\{n_c\}} \prod_{m=1}^{n_f} \binom{N_c(m)}{n_c(m)} (-1)^{(m-1)n_c(m)}, \quad (4)$$

with the constraint $\sum_m m n_c(m) = n_f$.

It will be demonstrated that it is feasible to evaluate exactly the weights (2),(4) even for a relative large number of impurity particles—results will be presented for $n_{b,f} \leq 32$ on a 32×32 lattice. For some observables the estimator $O_{i,\alpha}$ is independent of the cycle filling whereas in other cases the evaluation of its average may be more complicated. In some cases, it may be necessarily to carry out a separate sampling of the average estimator for each path. Here only the internal energy and the

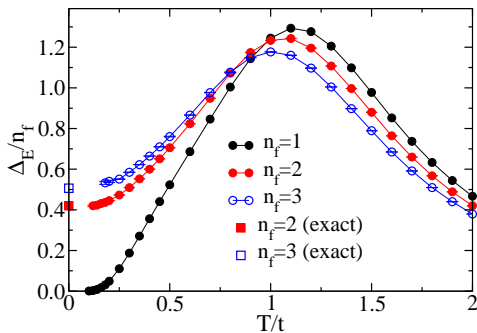


FIG. 3: (Color online) QMC and Lanczos results for the internal energy of a 4×4 system with $n_f = 1, 2, 3$ fermions, relative to the energy of the purely bosonic system.

phase stiffness will be considered, both of which have SSE estimators involving operator counts in P_i , which are independent of the distribution of A and B particles. The energy $E = \langle H \rangle$ is given simply by the average order p of the SSE Taylor expansion; $E = -\langle p \rangle / \beta$ [17]. The stiffness is the second derivative of the energy $E(\phi)$ with respect to a twist ϕ in the boundary condition. It is obtained by averaging the squared winding number [18, 19].

A limitation of the cycle summation approach is that the relative fluctuations in the weights $w_{b,f}$ grow as $n_{b,f}$ increases. Then only a decreasing subset of the generated configurations will contribute significantly to computed quantities. In addition, for fermions there is still a sign problem, although the summation over many cycle fillings with different signs does alleviate it significantly. These issues are illustrated and further discussed in Fig. 2. Another problem is that it becomes prohibitively time consuming to exactly evaluate $w_{b,f}$ for large $n_{b,f}$. For moderate $n_{b,f}$, it is possible to obtain results on large lattices in temperatures regimes where interesting physics takes place, as will be shown next.

Results.—The correctness of the QMC scheme was confirmed by exact diagonalization results for a 2×4 system at finite T . Even using momentum conservation, it is difficult to completely diagonalize a 4×4 system with two particle species. The ground state can be obtained using the Lanczos method, however.

An interesting quantity is the change $\Delta E(n_{b,f})$ in the internal energy relative to the $n_{b,f} = 0$ energy; $\Delta E = E(n_{b,f}) - E(0)$. Fig. 3 shows how QMC results for $\Delta E(n_f)/n_f$ approach corresponding Lanczos results for $n_f = 1, 2, 3$. Note that with $n_f = 1$, fermion anticommutation does not come into play and the same bosonic ground state as with $n_f = 0$ is obtained as $T \rightarrow 0$.

An effective interaction energy between impurities can be defined by subtracting the single-impurity result $\Delta E(1)$; $E_{\text{int}} = \Delta E(n_{b,f})/n_{b,f} - \Delta E(1)$. This quantity is shown in Fig. 4 for 8 bosonic and fermionic impurities in lattices of size $L = 8, 16$, and 32. At high temperatures $E_{\text{int}} < 0$, indicating effectively attractive interactions for both bosons and fermions. A singular behavior appears

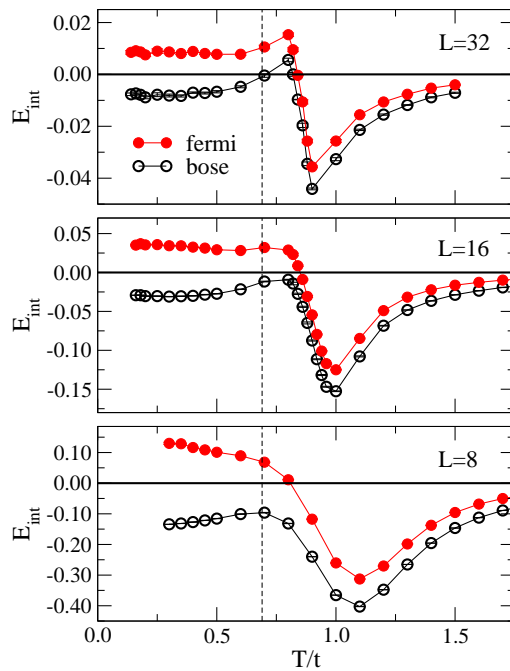


FIG. 4: (Color online) Interaction energy for 8 impurities in $L = 8, 16$, and 32 lattices. The dashed lines indicate T_{KT} .

to develop at $T \approx T_{KT}$, where for large systems both the fermionic and bosonic interactions first become increasingly attractive and then suddenly turn repulsive. At lower T the fermionic interactions stay repulsive while the bosonic ones become attractive again. The behavior is very similar for all impurity numbers $n_f \geq 2$ studied. In the case of fermions (bosons) E_{int} at low T increases as a function of n_f (decreases as a function of n_b), as would be expected for repulsive (attractive) interactions. When negative, E_{int} is seen to decrease as a function of the system size, indicating that the impurities do not demix but remain distributed throughout the system.

Note that n_f is fixed in Fig. 4, i.e., the impurity concentration decreases with increasing L . If the impurities do not segregate, it is clear that anticommutation dependent T at which fermions, at their typical separation, can begin to permute. Thus, the behavior around T_{KT} for a low impurity density should be a bosonic feature. The qualitative difference between bosonic and fermionic impurities emerges at lower temperature, where the fermions remain repulsive down to $T \rightarrow 0$ whereas the bosons become attractive [and eventually the effective interactions vanish as $E(n_b > 0) \rightarrow E(0)$ for bosons].

It appears likely that the singularity seen developing in Fig. 4 should move exactly to T_{KT} as $L \rightarrow \infty$ and, hence, that vortices play a decisive role in the effective interactions. One can speculate that the each impurity particle associates with a vortex. The low- T repulsive fermionic interactions may then point to vortex-antivortex pairs that increase in size and do not annihilate. There would

then be $n_f/2$ vortex-antivortex pairs left at $T = 0$.

The influence of the bosonic and fermionic impurities on the phase stiffness (the superfluid density [19]) around T_{KT} is almost indistinguishable for large system sizes, as shown for $L = 32$ in Fig. 5(a). In both cases the stiffness is mildly suppressed, pointing to a modest reduction in T_{KT} for impurity concentrations $1/32$ (16 impurities) and $1/16$ (32 impurities). However, as shown in Fig. 5(b), there are significant differences in the case of two impurities in a 4×4 lattice at low temperatures. As expected, for bosonic impurities the stiffness approaches that of the single-species system. Two fermions, on the other hand, strongly suppress the stiffness as $T \rightarrow 0$. In fact, $\rho_s \rightarrow -\infty$ as $T \rightarrow 0$, which can be traced to the minimum in the energy $E(\phi)$ as a function of the boundary twist ϕ being slightly away from $\phi = 0$. In addition to this anomaly, the ground state does not have momentum $q = 0$ but is degenerate with $\mathbf{q} = (\pm\pi/2, 0), (0, \pm\pi/2)$. These features suggest that the ground state is frustrated, which may again be indicative of the two fermions being tied to a vortex-antivortex pair. A drop in the stiffness is also seen for a small (2–4) number of fermions in larger lattices, at a T which decreases as L is increased for fixed n_f . The ground state may thus be insulating.

Summary and Conclusions.—The QMC method developed here enables studies of bosonic as well as fermionic impurity particles in a bath of hard-core bosons. Here a system with no interactions apart from the hard-core constraint was studied, but the method is applicable also in the presence of other interactions as long as they are equal for all species (inter- and intra-species).

In the model studied here, signs of a singular effective impurity interaction are seen at T_{KT} , pointing to a decisive role of vortices. At low T the effective fermionic interactions are repulsive whereas the bosonic ones are attractive. A scenario suggested by these findings is that impurities associate with vortices. An effectively repulsive fermionic impurity interaction, along with a drop observed in the phase stiffness, would then imply that some vortex-antivortex pairs remain as $T \rightarrow 0$, potentially leading to an insulating ground state. For bosonic impurities, the ground state is the same as without impurities. Future studies will address correlations in systems with a very small number of impurities at lower temperatures. This should give further insights into the nature of the ground state of the bose-fermi mixture.

In the presence of a trapping potential, the repulsive fermions should be expelled to the condensate boundary at low temperatures. However, simulations of the grand-canonical ensemble, but with fixed n_f , demonstrate an effectively attractive fermi-bose interactions (the filling $\langle n \rangle$ becomes larger than $1/2$). Thus the boundary should be in an interesting non-trivial mixed state.

I would like to thank Anatoli Polkovnikov and Asle Sudbø for useful discussions. This work was supported by the NSF under grant No. DMR-0513930.

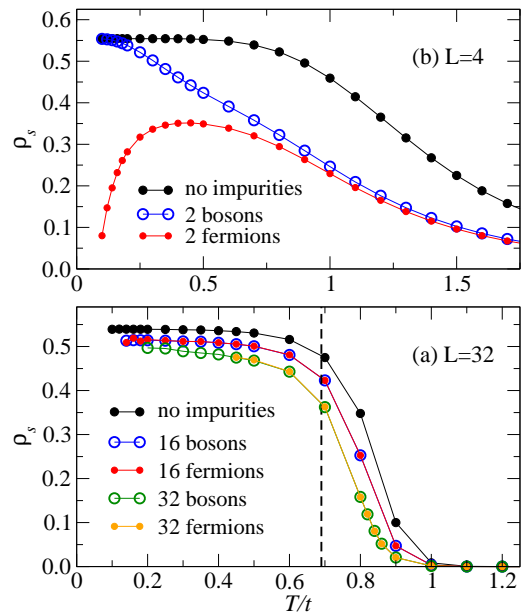


FIG. 5: (Color online) Phase stiffness for (a) $L = 4$ systems with $n_{b,f} = 0, 2$ and (b) $L = 32$ systems with $n_{b,f} = 0, 16, 32$.

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- [1] I. Bloch, J. Dalibard, and W. Zwerger, arXiv:0704.3011 (to appear in Rev. Mod. Phys.).
 - [2] W. Hofstadter, J. I. Cirac, P. Zoller, E. Demler, and M. D. Lukin, Phys. Rev. Lett. **89**, 220407 (2002).
 - [3] H. P. Büchler and G. Blatter, Phys. Rev. Lett. **91**, 130404 (2003).
 - [4] K. Sengupta, N. Dupuis, and P. Majumdar, Phys. Rev. A **75**, 063625 (2007).
 - [5] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A **68**, 023606 (2003).
 - [6] L. Mathey, S.-W. Tsai, and A. H. Castro Neto, Phys. Rev. Lett. **97**, 030601 (2006).
 - [7] M. Lewenstein, L. Santos, M. A. Baranov, and H. Fehrmann, Phys. Rev. Lett. **92**, 050401 (2004).
 - [8] K. Günter *et al.*, Phys. Rev. Lett. **96**, 180402 (2006); S. Ospelkaus *et al.*, *ibid.*, **96**, 180403 (2007).
 - [9] A. Truscott *et al.*, Science **291**, 2570 (2001).
 - [10] A. Imambekov and E. Demler, Phys. Rev. A **73**, 021602(R) (2006).
 - [11] K. Harada and N. Kawashima Phys. Rev. B **55**, R11949 (1998).
 - [12] D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).
 - [13] J. E. Hirsch, R. L. Sugar, D. J. Scalapino and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).
 - [14] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, Zh. Eks. Teor. Fiz. **114**, 570 (1998) [JETP **87**, 311 (1998)].
 - [15] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002).
 - [16] M. Boninsegni, N. Prokof'ev, and B. Svistunov, Phys. Rev. Lett. **96**, 070601 (2006).
 - [17] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991); A. W. Sandvik, J. Phys. A **25**, 3667 (1992).
 - [18] A. W. Sandvik, Phys. Rev. B **56**, 11678 (1997).
 - [19] E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987).